

Supplementary Information

New cyclometalated Ir(III) complexes with NCN pincer and meso-phenylcyanamide BODIPY ligands as efficient photodynamic therapy agents

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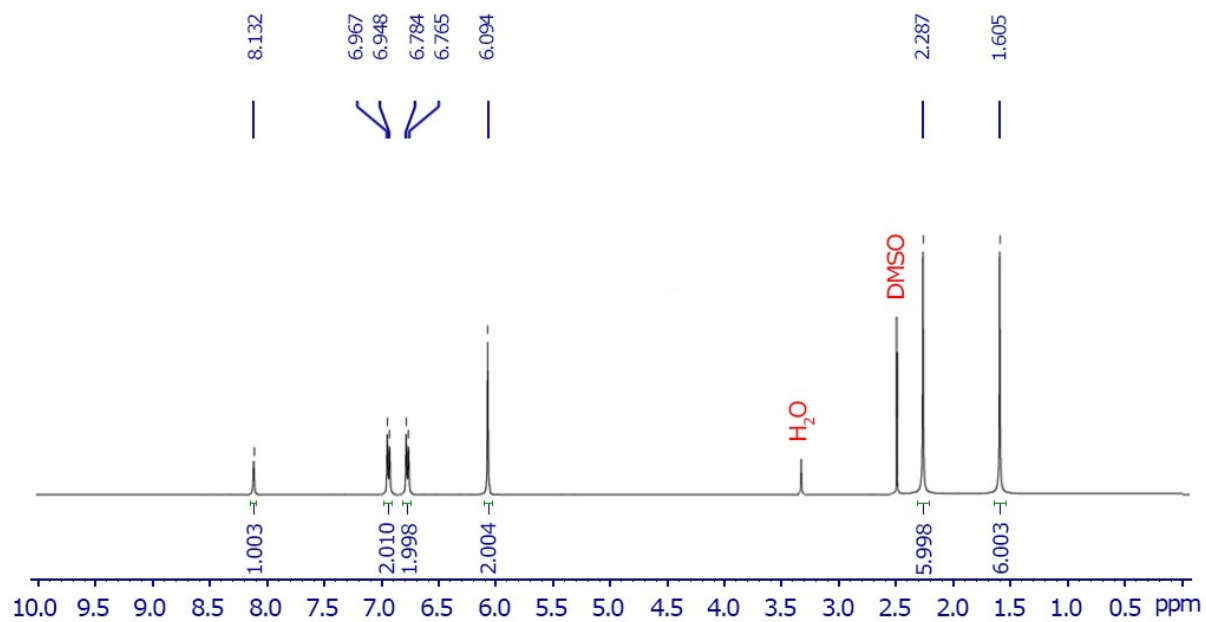


Fig. S1. ^1H NMR spectrum of ligand Pcyd-BODIPY ($\text{DMSO-}d_6$).

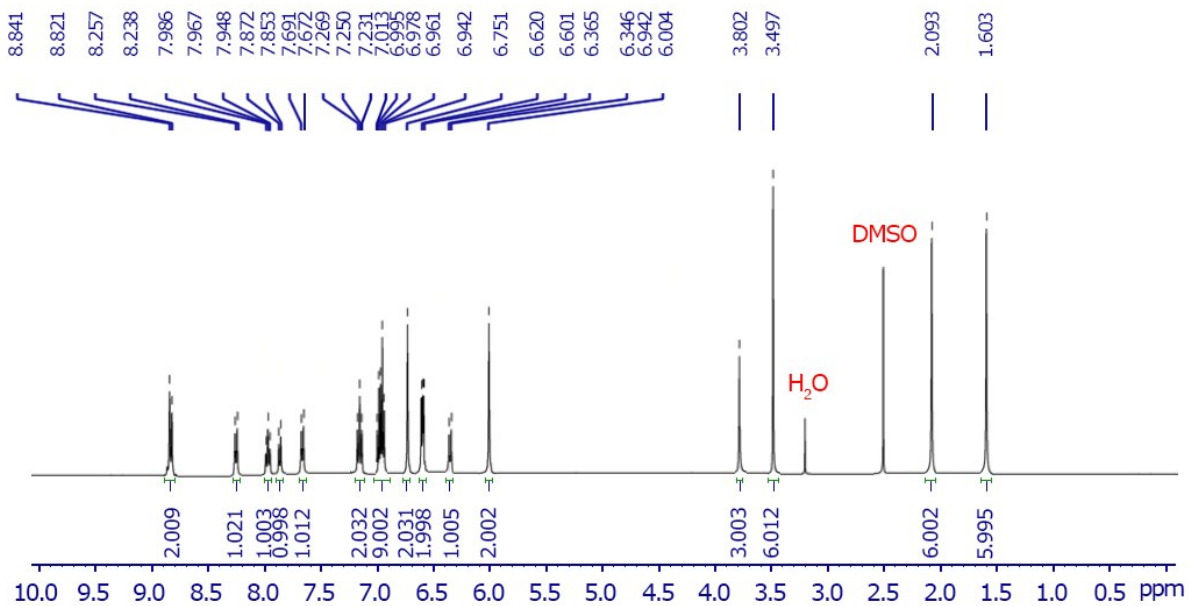


Fig. S2. ¹H NMR spectrum of complex **1** (DMSO-*d*₆).

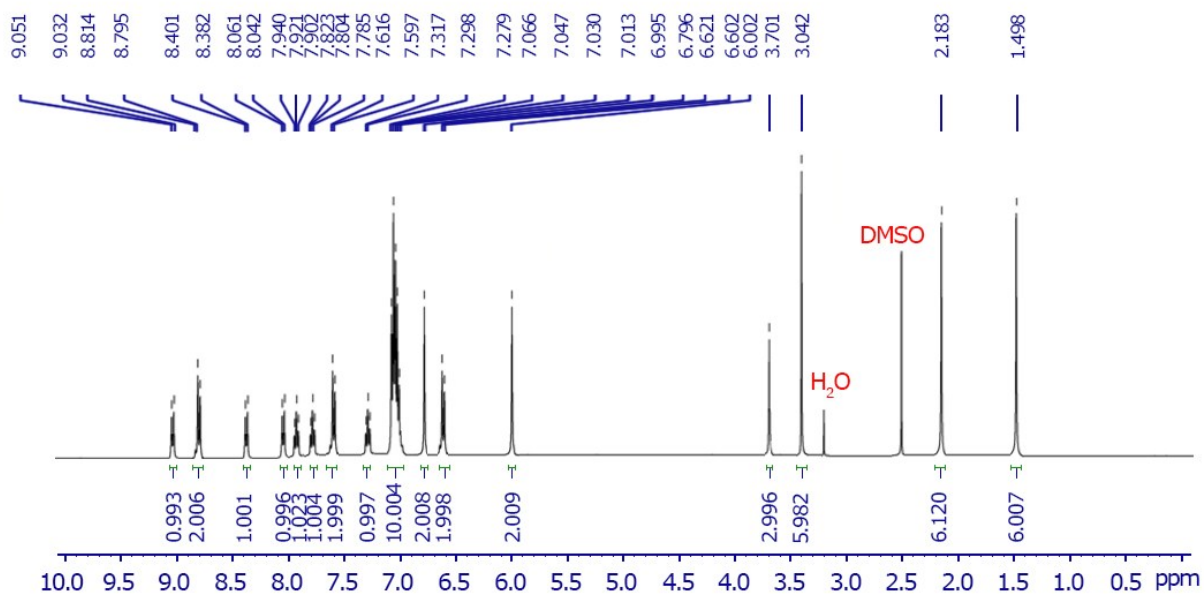


Fig. S3. ¹H NMR spectrum of complex **2** (DMSO-*d*₆).

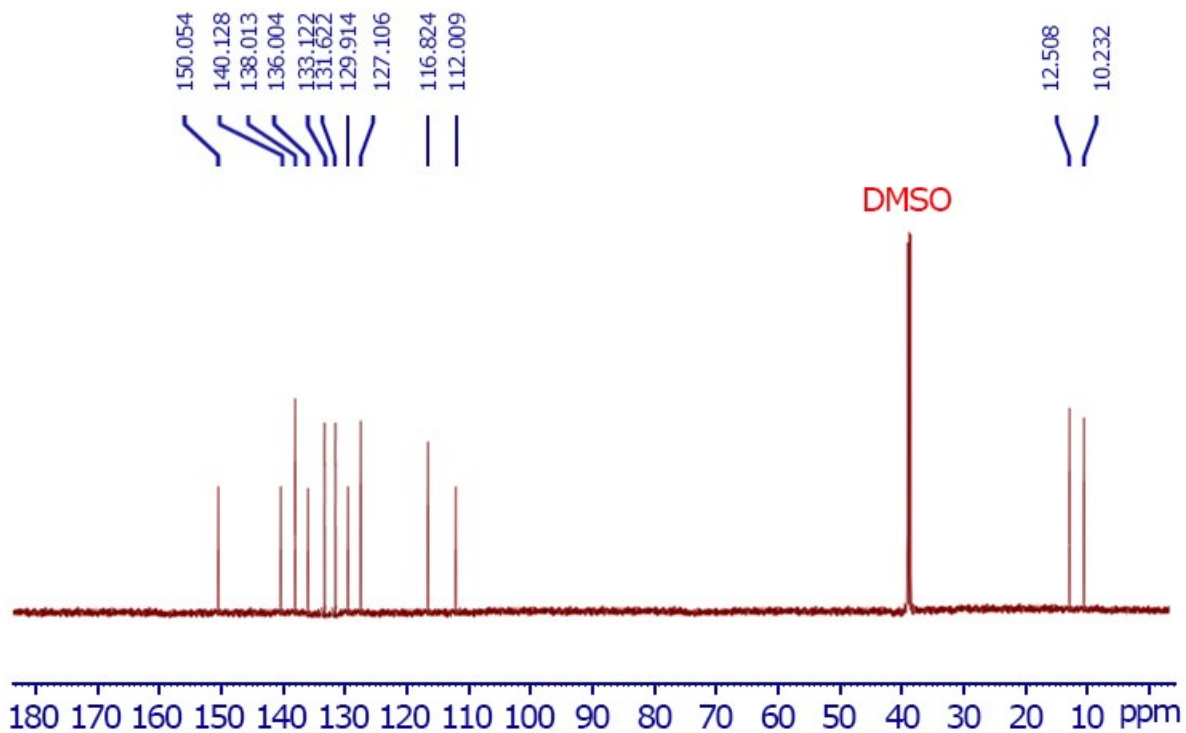


Fig. S4. ^{13}C NMR spectrum of ligand Pcyd- BODIPY ($\text{DMSO-}d_6$).

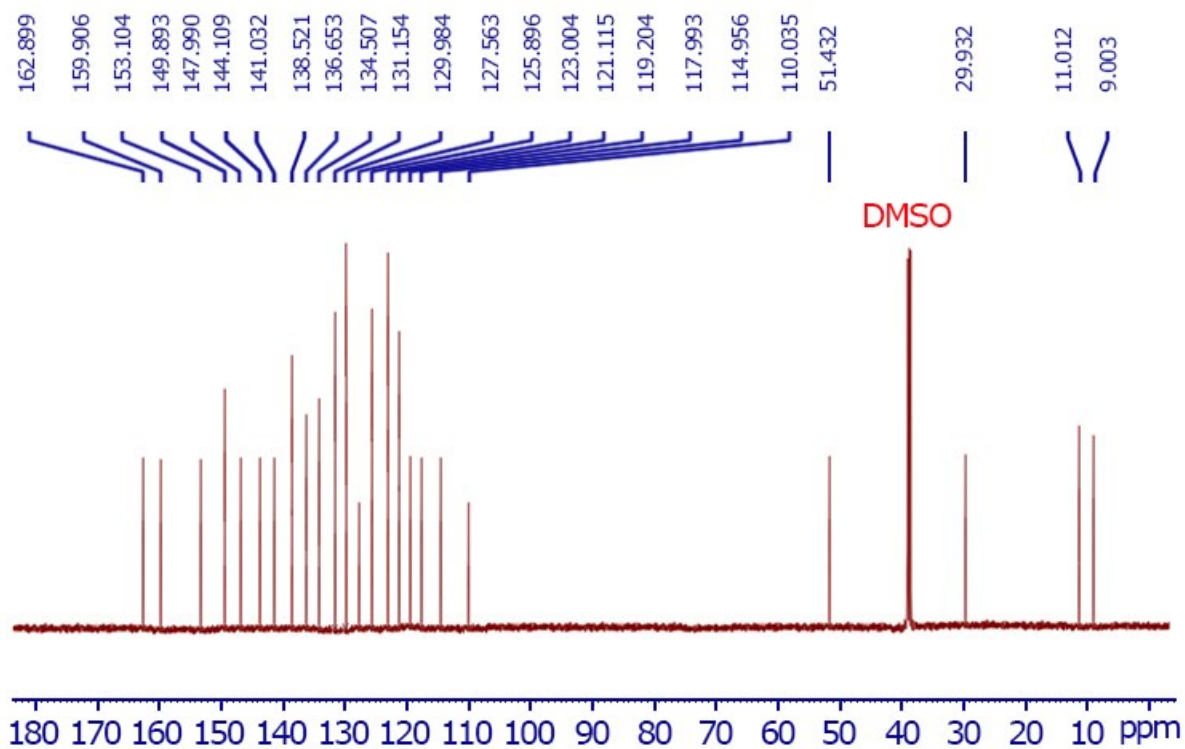


Fig. S5. ^{13}C NMR spectrum of complex **1** ($\text{DMSO-}d_6$).

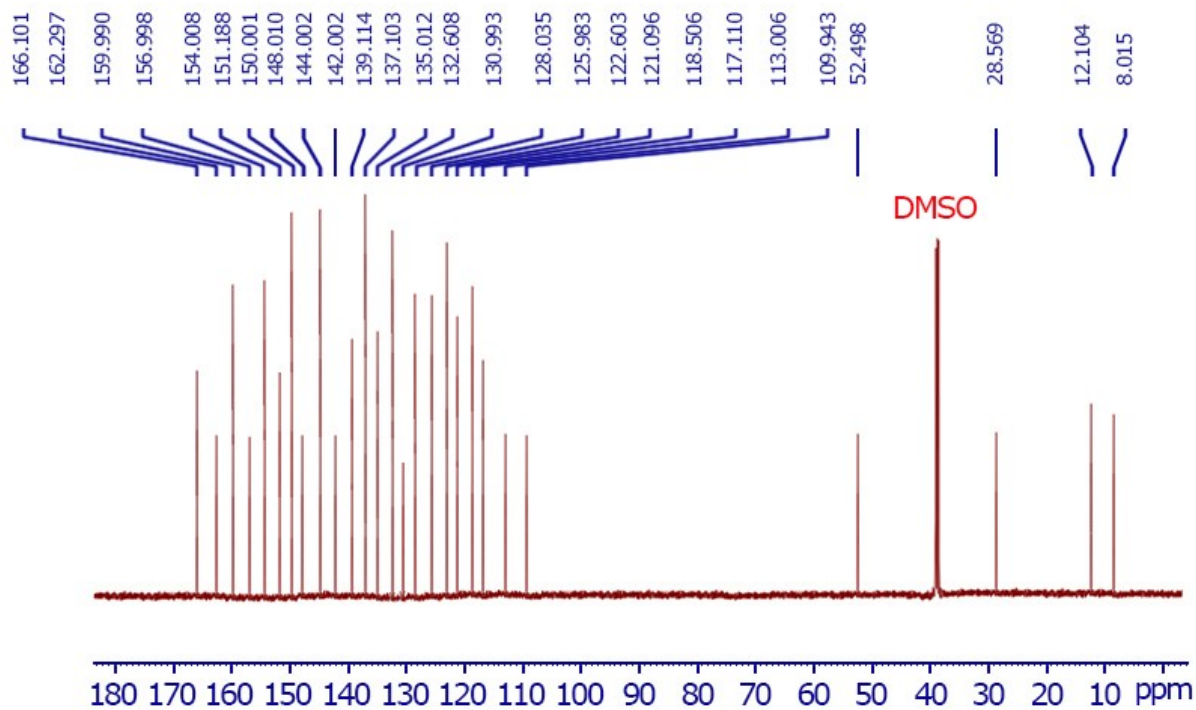


Fig. S6. ^{13}C NMR spectrum of complex **2** ($\text{DMSO-}d_6$).

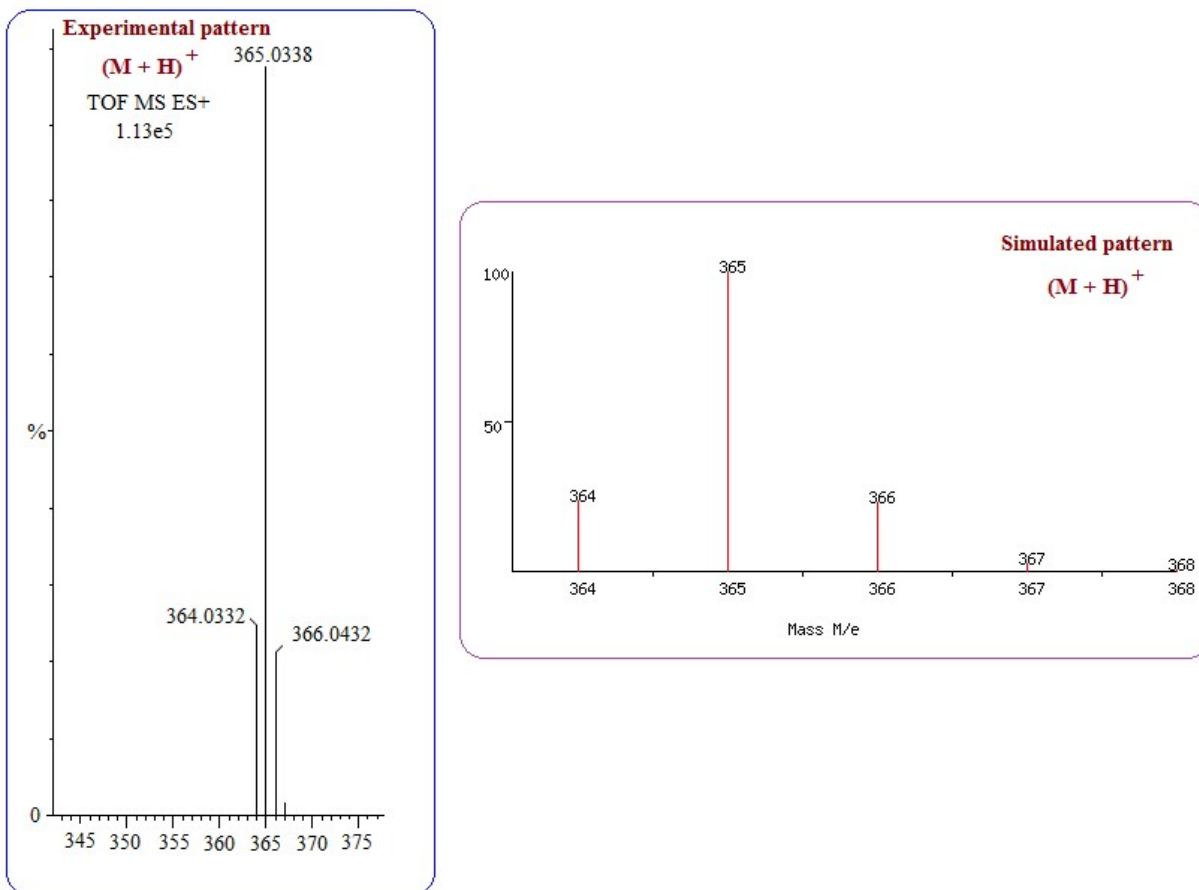


Fig. S7. TOF MS spectrum of ligand Pcyd- BODIPY.

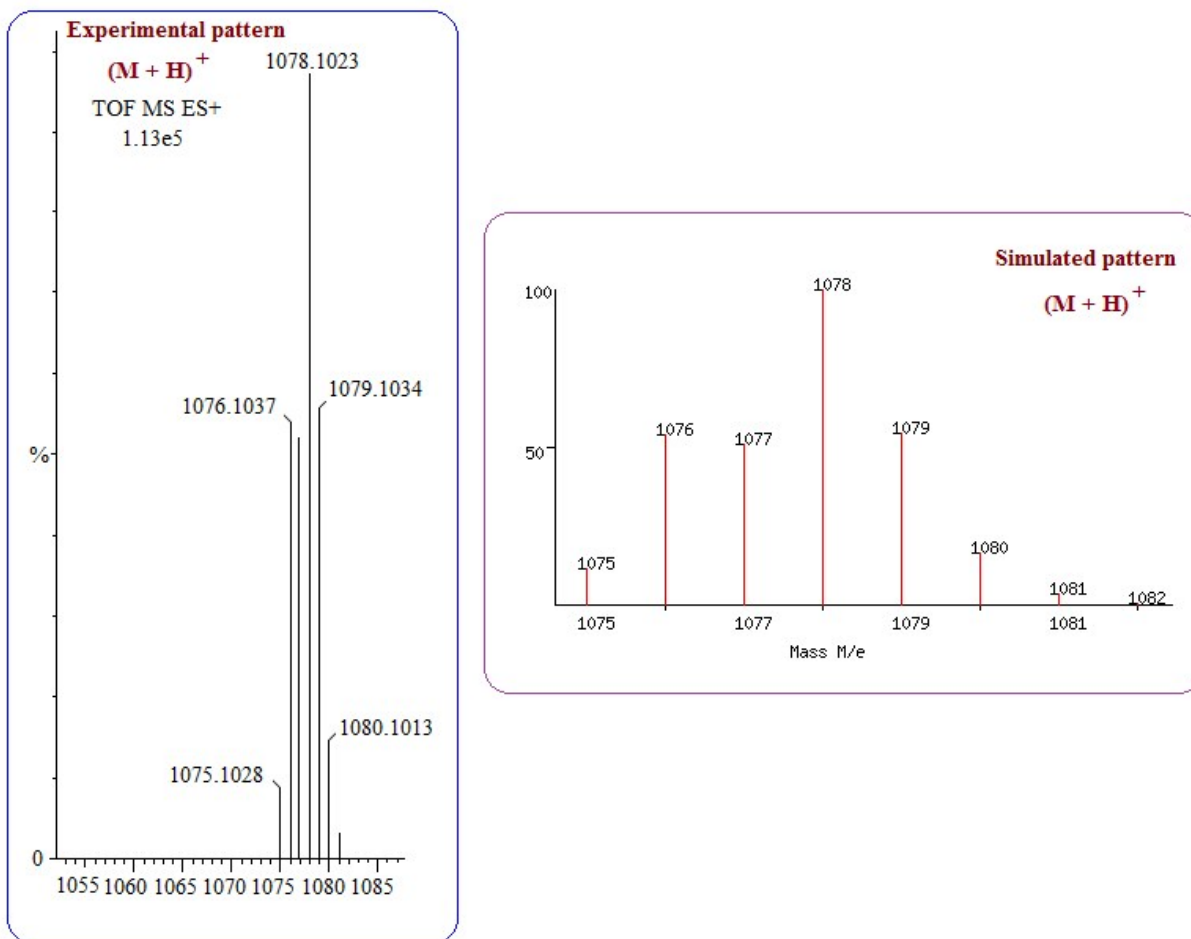


Fig. S8. TOF MS spectrum of complex 1.

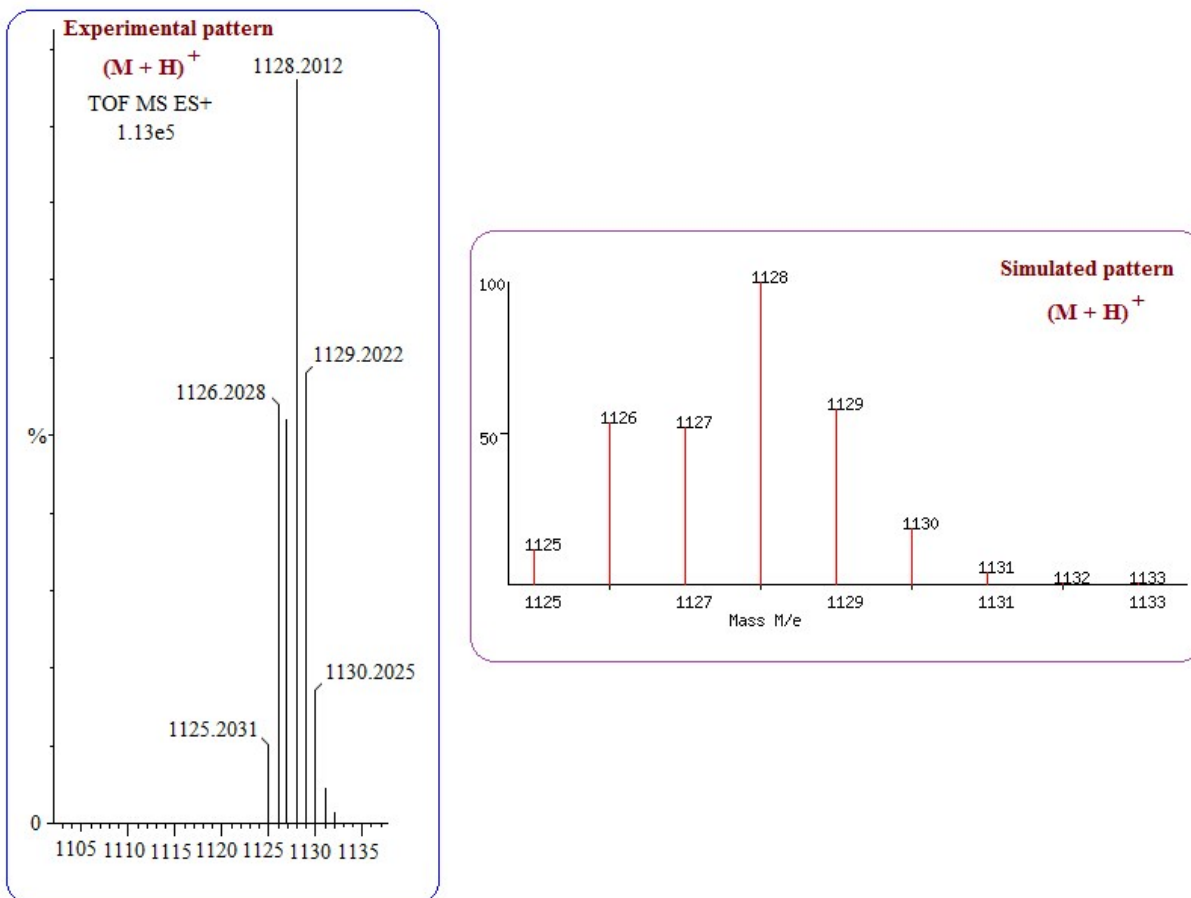


Fig. S9. TOF MS spectrum of complex 2.

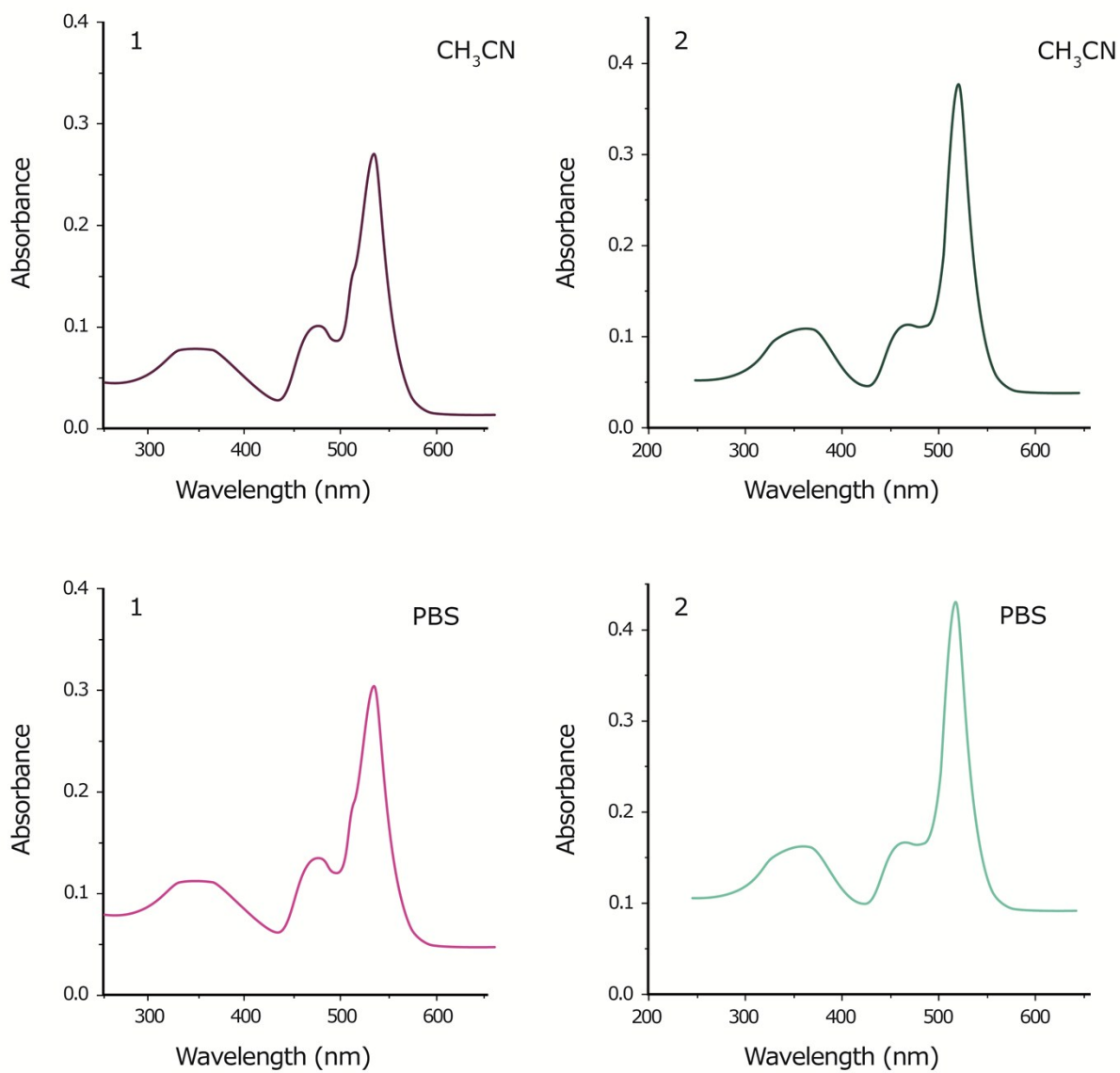


Figure. S10. UV/Vis spectra of complexes **1** and **2** in CH₃CN and PBS at 298 K.

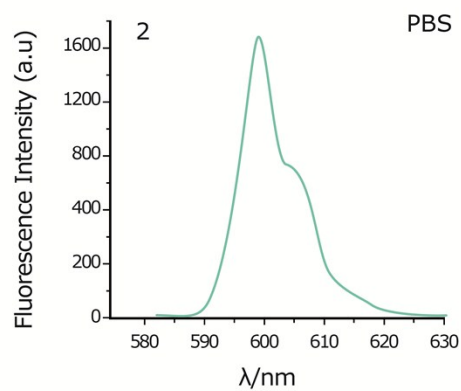
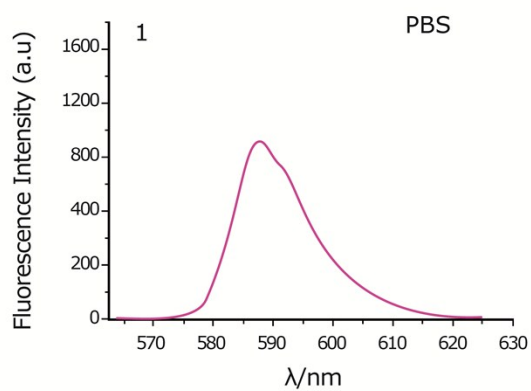
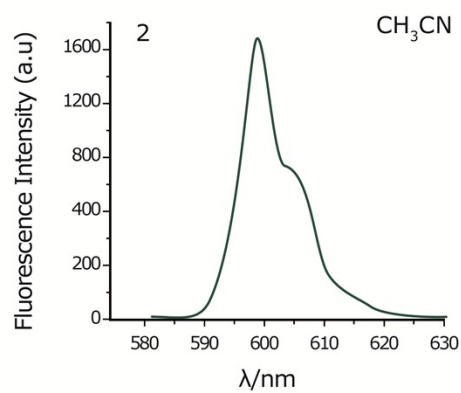
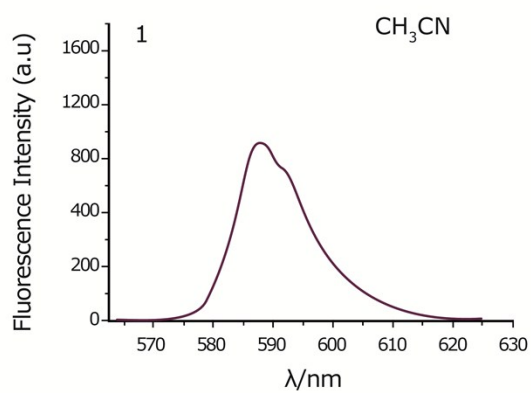


Figure. S11. Emission spectra of complexes **1** and **2** in CH₃CN and PBS at 298 K.

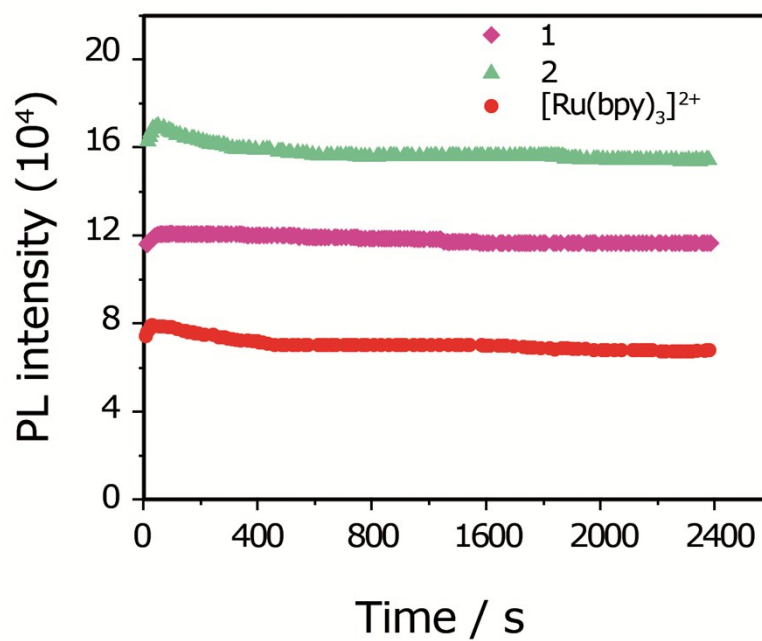


Figure. S12. Photobleaching fluorescent intensity of complexes **1** and **2** under continuous irradiation (500 nm) in Tris-HCl buffer (5 mM Tris, 50 mM NaCl, pH = 7.4).

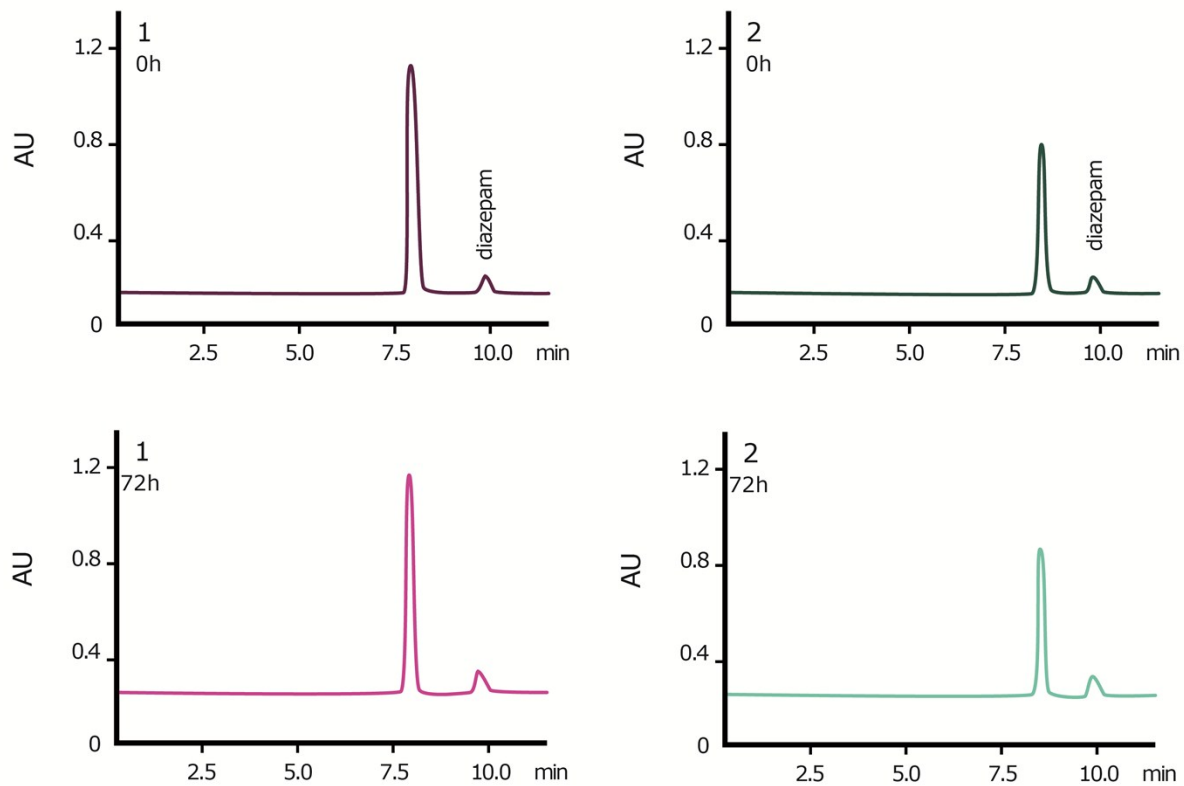


Fig. S13. LC-UV traces of plasma incubated with complexes **1** and **2** (20 μ M, 37 $^{\circ}$ C) at t = 0 and 72 h. (Diazepam was used as internal standard).

Table S1. Photophysical data of complexes **1** and **2**.

Complex	UV/Vis λ [nm]	Emission ^[a] λ [nm]	(Φ_{em}) ^[b]	Lifetimes [ns] ^[c]
1	ACN: 350, 477, 541	ACN: 588	1.98	702
	PBS: 349, 478, 543	PBS: 587		
2	ACN: 358, 463, 526	ACN: 598	2.13	728
	PBS: 355, 465, 528	PBS: 599		

[a] Emission spectra recorded in ACN (acetonitrile).

[b] Φ_{em} refers to the luminescence quantum yield and were calculated according to literature procedures. *

[c] Lifetimes evaluated ACN (acetonitrile).

* G. A. Crosby and J. N. Demas, *J. Phys. Chem.* 1971, **75**, 991-1024.

Table S2. Singlet oxygen quantum yields upon irradiation at 500 nm.

	1	2
PBS (indirect)	2%	3%
ACN (direct)	79%	92%
ACN (indirect)	72%	88%

Table S3. Ratio of peak areas of complex/diazepam

	1	2
t = 0 h	8.92	9.58
t = 72 h	8.88	9.52